

Confinement and Deconfinement of Spinons in Two Dimensions

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Spinons are emergent fractional (spin-1/2) excitations of quantum magnets. While they are well established and understood in one dimension, characterizing them in two-dimensions, in theoretical models and real materials, has been challenging. Here we use Monte Carlo methods to study spinons in a resonating valence-bond (RVB) spin-liquid, as well as in a model which can be tuned from an antiferromagnet to a valence-bond solid (VBS); a crystal of singlets. We use a generalized valence-bond basis to compute the intrinsic size λ of an individual spinon and the size Λ of a bound state. We confirm that spinons are deconfined, $\Lambda \rightarrow \infty$ and λ finite, in the RVB. In the VBS $\lambda > \Lambda$, i.e., the spinon is soft and shrinks as the bound state is formed. Both λ and Λ diverge at the VBS–antiferromagnetic critical point. We conclude that the spinon deconfinement is marginal in the lowest-energy state in the spin-1 sector, due to weak attractive spinon-spinon interactions. Deconfinement should occur at higher energies.

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The concept of *confinement* originated in particle physics, where quarks are bound into hadrons by “gluon strings”, leading to a distance-independent force and the inability to isolate individual quarks [1]. This picture has been carried over to condensed matter physics as well. One example is the non-magnetic valence-bond-solid (VBS) state of a two-dimensional (2D) quantum spin system, whose ground state consists of a crystalline arrangement of two-spin singlets (valence bonds). An elementary excitation corresponds to promoting one bond into a triplet. The members of this triplet (the spinons) stay bound to each other, due to a string of misaligned singlets forming when separating the spinons [2]. In a one-dimensional (1D) VBS the confining string does not exist, as there is no medium surrounding the phase-shifted dimers between the spinons. The spinons then deconfine and become independent elementary excitations. The spinon concept was originally introduced as a spin analog [3] of the fractional excitations of conjugated polymers [4], which are phase-twist solitons—domain walls between two out-of-phase dimerized chain segment.

An ongoing quest in quantum magnetism is to identify 2D systems in which spinons can deconfine. Deconfinement and weak confinement of spinons have been experimentally observed in one dimensional (1D) spin chains [5] and ladders [6], respectively, by neutron scattering. Deconfinement is characterized by a broad continuum of spin-1 excitations. These observations and conclusions are aided by the known triplet spectrum [7] of the Heisenberg chain, where the existence of spinons is understood rigorously [8]. For 2D systems, this way of detection is difficult, due to a lack of established model spectral functions for spinons and the existence of significant continua even in the magnon spectrum of antiferromagnets [9]. While alternative experimental methods have also been proposed [10], this remains a challenging issue. In numerical model studies, correlations of excess magnetization with impurities [11, 12] and other inhomogeneities

[13] have been used to study spinons.

Here we use a quantum Monte Carlo (QMC) approach for homogeneous systems [14] and address the mechanism of 2D spinon deconfinement promoted by Senthil *et al.* [15–17]. In their picture, a spinon in a square-lattice VBS can be viewed as vortex at the nexus of four VBS domains, with the core carrying spin-1/2. These vortices bind with anti-vortices to form the gapped spin-1 triplons. The binding potential weakens as the fluctuations of the VBS increase and a *deconfined quantum-critical* (DQC) point is approached which separates the VBS from the standard antiferromagnetic (Néel) state.

Deconfined spinons are expected in spin liquids, which are non-magnetic states with no broken symmetries [18]. The DQC point is an isolated, gapless (algebraic) spin liquid. In the near-DQC VBS, the triplon is predicted to become large, exceeding the correlation length [16, 17], and may be regarded as loosely bound spinons. Several QMC studies of J - Q models, where the Heisenberg exchange is supplemented with higher-order interactions [19], support the existence of an unusual critical point [19–23] and the critical thermodynamic properties are also consistent with spinons [24].

Objectives and Findings—We study properties of the DQC spinons and their near-DQC bound states in the 2D J - Q model. Computing the spinon size and confinement length, we demonstrate that a naive picture of a large bound state of two small objects fails—the spinons themselves are of size comparable to the bound state and are “soft”, shrinking when forming bound states. This differs from the prototypical short-bond resonating valence-bond (RVB) spin liquid [25, 26], which we also study as a point of reference. Here the deconfined spinons are small, with radius of a few lattice spacings.

Methods—In Ref. [14] we showed how spinons can be characterized for bipartite systems in the valence-bond (singlet) basis extended to $S = 1/2$ and $S = 1$ by introducing one (on a lattice with an odd number of sites)

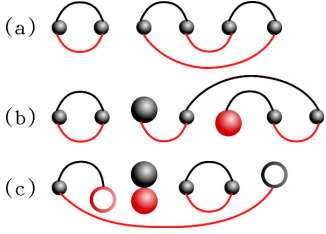


FIG. 1: (Color online) Transition graphs for $S = 0$ (a), $S = 1/2$ (b), and $S = 1$ (c). The bonds and larger circles indicate valence bonds and unpaired (\uparrow) spins, respectively, in ket (black) and bra (red) states. The statistics of separation of unpaired spins in (b) and (c) can be used to characterize the spatial properties of spinons and their bound states.

or two (for an even number of sites) unpaired spins. An $S = 0$ state is a superposition of states $|V_N\rangle$ in which all N spins are paired up into $N/2$ singlets between sublattice A and B sites, while for $S = 1/2$ and $S = 1$ the basis states are, respectively, $|V_{N-1}\rangle \otimes |\uparrow_a\rangle$ and $|V_{N-2}\rangle \otimes |\uparrow_a\rangle \otimes |\uparrow_b\rangle$, where a and b are sites on different sublattices [27, 28]. Superpositions can be generated probabilistically either in variational states (amplitude-product states [29] and their generalizations [30]) or in QMC simulations of Hamiltonians. Examples of configurations are shown in Fig. 1. We use the formulation of the projector QMC method discussed in Ref. [31].

The valence-bond basis being overcomplete and non-orthogonal, one should not consider the unpaired spins directly as spinons. However, as shown in Ref. [14], to which we refer for details, the statistics of the separation of unpaired spins in transition graphs (see Fig. 1) are related to wave-function overlaps and can be used to extract the intrinsic size of a single spinon as well as the size of an $S = 1$ bound state. We denote the probability distribution between \uparrow spins in the bra and ket state of an $S = 1/2$ configuration $P_{AA}(r)$ and between those on different sublattices in an $S = 1$ state by $P_{AB}(r)$. The former contains information on the spinon size and the latter on the bound state (or lack thereof). The same information is contained also in the difference $C(r) = C_S(r) - C_0(r)$ between the z -component spin-spin correlation function in the $S = 1/2, 1$ and $S = 0$ states [14]. The method of statistics of separations is easier, since $C(r)$ is statistically noisy for large systems. The latter method can, however, be extended to non-bipartite systems and other computational methods.

Models—We use Monte Carlo sampling [29] to generate valence-bond configurations for the short-bond RVB, as done in two recent studies to characterize its spin and dimer correlations [32, 33]. We use the RVB as a reference point for an established $U(1)$ spin liquid. It is expected to have deconfined spinons but their spatial characteristics have not been considered before, to our knowledge. Our main interest is to characterize spinons at the Néel–VBS transition of the J - Q model. Here we consider a Q -term consisting of three singlet projectors

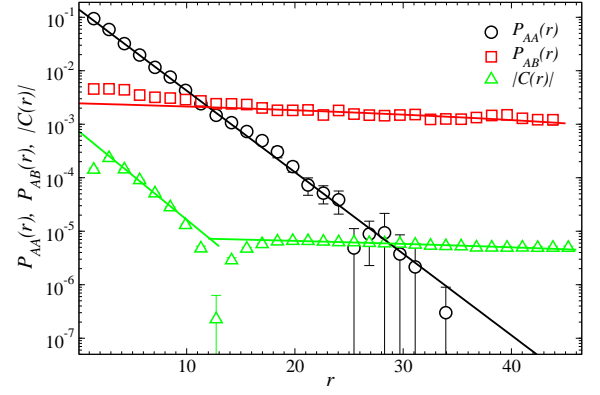


FIG. 2: (Color online) Spinon distributions and correlations along the diagonal lattice direction of the RVB spin liquid. Black and red circles show the single-spinon overlap $P_{AA}(r)$ in an $S = 1/2$ state on a 65×65 lattice. The exponential decay (fitted line) gives the spinon size $\lambda = 2.96(1)$ lattice spacings. Red squares show the two-spin distribution $P_{AB}(r)$ in the $S = 1$ state on a 64×64 lattice, fitted to $\sim 1/r^\alpha$ with $\alpha \approx 0.6$. The green triangles show the difference $C(r)$ between the spin correlations in the $S = 1$ and $S = 0$ systems. This quantity exhibits both a spinon-size effect (exponential short-distance decay) and deconfinement (weak power-law decay at long distances). There is a phase shift at $r \approx 9\sqrt{2}$.

$C_{ij} = 1/4 - \mathbf{S}_i \cdot \mathbf{S}_j$. The Hamiltonian is [21]

$$H = -J \sum_{\langle ij \rangle} C_{ij} - Q_3 \sum_{\langle ijklmn \rangle} C_{ij} C_{kl} C_{mn}, \quad (1)$$

where $\langle ij \rangle$ and $\langle ijklmn \rangle$ denote, respectively, nearest neighbors and three nearest-neighbor pairs in horizontal or vertical columns on the square lattice. The critical coupling ratio separating the Néel and VBS phases is $g_c = (Q_3/J)_c \approx 1.50$ [21], and for large g the VBS order is very robust.

We also study the 1D J - Q_3 model including static dimerization, with different couplings on even and odd bonds;

$$H = - \sum_{i=\text{even}} (J_1 C_{2i,2i+1} + J_2 C_{2i+1,2i+2}) - Q_3 \sum_i C_{i,i+1} C_{i+1,i+2} C_{i+2,i+3}. \quad (2)$$

When $J_1 = J_2$ the quasi-ordered to VBS transition (which is of the same kind as in the frustrated Heisenberg chain [34]) is at $Q_3/J = 0.1645$ [14]. In this study we use this critical ratio and tune $\rho = J_2/J_1$. The explicit dimerization introduced by $\rho \neq 1$ leads to confinement [12], while the spinons are deconfined when $\rho = 1$. We will demonstrate similarities with the 2D J - Q_3 model.

RVB Spin Liquid—RVB spin liquids have been considered as promising candidates for explaining high temperature superconductivity in cuprates when doped [25, 35]. It is therefore also interesting to examine in detail properties of the insulating host system. Recently, it was found

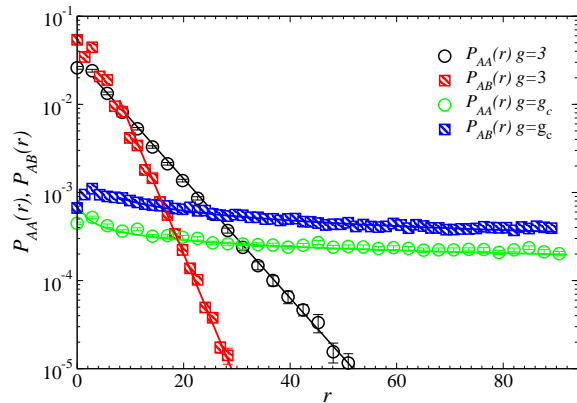


FIG. 3: (Color online) Spinon distributions for the 2D J - Q_3 model on $L = 128$ and 129 lattices at $g = 3$ (VBS) and $g_c = 1.5$ (critical). The lines are exponential fits for the $g = 3$ VBS, giving the single-spinon size $\lambda = 6.4$ extracted from $P_{AA}(r)$ in the $S = 1/2$ state and the confinement length $\Lambda = 3.1$ extracted from $P_{AB}^*(r)$ in the $S = 1$ state. Both lengths diverge as $g \rightarrow g_c$, where the distributions decay algebraically.

that the simplest equal-amplitude short-bond RVB is a quantum-critical VBS, with exponentially decaying spin correlations but power-law dimer correlations [32, 33]. It has been long expected that the RVB hosts deconfined spinon excitations [18].

The parent Hamiltonian of the short-bond RVB was found recently [36]. Although the $S = 1/2$ and $S = 1$ states we study here may not be its exact lowest states in these sectors, one can still expect them to be good variational states—the actual excitations of the Cano-Fendley Hamiltonian should be very similar.

We characterize the spinons in Fig. 2. The $S = 1/2$ distribution $P_{AA}(r)$ demonstrates a well-defined intrinsic spinon wave packet, decaying as $e^{-r/\lambda}$ with the spinon size $\lambda = 2.96(1)$. The $S = 1$ distribution $P_{AB}(r)$ is peaked at short distances and appears to decay as $r^{-\alpha}$ with $\alpha \approx 0.6$. This implies marginal deconfinement due to weak attractive spinon-spinon interactions. In Fig. 2 we also show that the length-scales observed in $P_{AA}(r)$ and $P_{AB}(r)$ are manifested in the correlation function $C(r)$ as well. Hence, the distributions do capture actual physical, basis-independent length-scales [14].

J-Q model—The Néel-VBS transition has been debated for years [2]. In 2004, Senthil et al. presented a scenario encompassing several earlier works [2, 37, 38] and further proposed a mechanism leading to a generic continuous transition [15–17]. This scenario is at odds with the “Landau Rule” according to which transitions between the two ordered states should be first-order. A key aspect of the theory is that both order parameters arise out of spinons, which condense in the Néel state and confine in the VBS (where valence bonds can be regarded as tightly bound spinon pairs). Exactly at the DQC point separating the ordered states the spinons should deconfine. Although opposing views have been

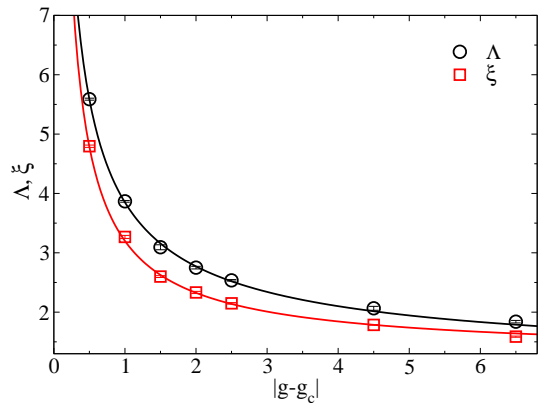


FIG. 4: (Color online) Divergent behavior of the correlation length ξ and the confinement length Λ as the coupling ratio approaches the critical point ($g_c = 1.50$) of the J - Q_3 model. The curves are fits to the power-laws discussed in the text.

put forward [39–41], the generic continuous nature of the Néel-VBS transition has support in QMC studies of J - Q [19, 21, 22, 31] and other [20] models, including a predicted emergent $U(1)$ symmetry reflecting the gauge structure of the theory, where spinons interact with an $U(1)$ gauge field, as described by the non-compact CP^1 field theory.

The DQC scenario motivates us to investigate spinons directly, by computing the spinon size λ and the confinement length Λ in VBS states and approaching the critical point. As shown in Fig. 3, both $P_{AA}(r)$ and $P_{AB}(r)$ are exponentially decaying in the VBS phase, with $\lambda = 6.4(1)$ and $\Lambda = 3.1(1)$ at $g = 3$. Surprisingly, the intrinsic size of a single spinon is, thus, much larger than the bound state of two spinons. We interpret this as a softness of the spinon, which causes it to shrink when subject to attractive interactions from an anti-spinon. This should be a signature of the vortex-nature of the spinon, as the opposite circulations of the members of the pair should lead to cancellations away from the double-vortex core. Such shrinkage of vortices can also occur under certain conditions in superconductors [42, 43].

Approaching the critical point both λ and Λ diverge, and at the critical point power laws $P_{AA}(r) \sim 1/r^\alpha$ and $P_{AB}(r) \sim 1/r^\beta$ obtain, with $\alpha \approx \beta = 0.3 \pm 0.1$. In the DQC theory it is predicted that the divergence of Λ should be faster than the correlation length ξ ; $\Lambda \propto \xi^{1+k}$, with $k > 0$ and less than the exponent governing the rate of divergence of the cross-over length-scale of the emergent $U(1)$ symmetry (which should be the longest length-scale in the system close to the DQC point) [16]. We extract ξ from spin-spin correlations. The length-scales ξ and Λ are graphed versus the coupling ratio in Fig. 4. Using lattice sizes L up to 128, we can reliably extract Λ and ξ when they are roughly less than 10—beyond which the size-dependence becomes significant and extrapolating to infinite size is difficult. Although we can therefore not reach far into the asymptotic scaling

regime, the dependence on $g - g_c$ is still consistent with the expected power-law divergence, if we allow a constant correction, i.e., fitting to the forms $\Lambda = a + b(g - g_c)^{-\mu}$ and $\xi = a + b(g - g_c)^{-\nu}$. We then find $\mu = 0.7(1)$ and $\nu = 0.8(1)$. The correlation-length exponent $\nu = 0.60(2)$ was obtained in Ref. [22] based on finite-size scaling collapse for larger systems in the close neighborhood of the critical point. The results based on Fig. 4 may be affected by further non-asymptotic corrections. Regardless of the precise values of μ and ν , it is clear that $k = \mu/\nu - 1$ is very close to 0. This is consistent with the value 0.2(1) obtained in Ref. [21] for the exponent governing the $U(1)$ to Z_4 cross-over.

1D deconfinement—In the 1D VBS phase, without enforced dimerization, $J_1 = J_2$ in Eq. (2), the spinons are small and deconfined, as shown in Ref. [14]. By turning on a symmetry-breaking dimerization, $\rho = J_2/J_1 > 1$, one can tune the confinement length from arbitrarily large to arbitrarily small (as will be discussed elsewhere [44]). Here, to compare with the 2D model approaching its critical point, we instead show results for $g = Q_3/J$ fixed at the critical value $g_c = 0.1645$ when $J_1 = J_2$. Keeping $g = g_c$ and turning on the static dimerization, $\rho > 1$, we observe in Fig. 5 that $\Lambda \approx \lambda$ (Λ being slightly larger), with both lengths diverging as $\rho \rightarrow 1$. This is similar to the behavior observed in the 2D model (apart from the lack of spinon shrinkage). Thus, *the fact that the spinon size and the confinement length are both divergent does not invalidate the deconfinement picture*. At the critical point, the 1D “spinon shape” distribution $P_{AA}(r)$ also decays as a power-law, while the pair distribution $P_{AB}(r)$ is peaked at the longest distance, reflecting marginal (critical) spinons subject to weak repulsive interactions [14]. The main difference in the 2D model is that the effective spinon-spinon interactions are attractive, not only in the VBS phase but also at criticality.

Conclusions—We showed that a spinon in the 2D J - Q_3 model shrinks when a bound-state (triplon) is formed. This is most likely a generic aspect of VBS states; a consequence of the vortex nature [17] of the spinons. We should stress here that the reason why the vortices do not annihilate is that we restrict the system to the $S = 1$ sector, while spinon annihilation would bring it back to the $S = 0$ ground state. Both the spinon size and the confinement length diverge as the critical VBS–Néel point is approached, and at the critical point the distribution functions decay as power laws. This is also necessary for continuity, because in the Néel state both distributions become flat (as we discussed for 1D systems in Ref. [14] and have also verified in 2D), when the spinons completely lose their identity as individual objects.

Our scenario deviates from a simple picture of the near-critical triplon being a large object formed by two small particles. The question then is: Are the spinons nevertheless deconfined, independently propagating excitations? We showed with a known example that in 1D that

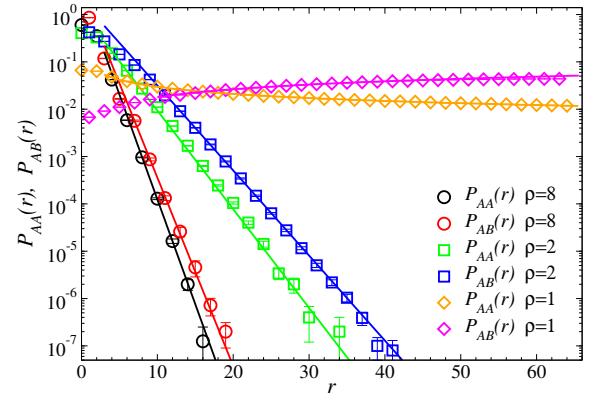


FIG. 5: (Color online) Spinon statistics of the J_1 - J_2 - Q_3 chain with $Q_3/J_1 = 0.1645$ (the critical point when $J_1 = J_2$) for three ratios $\rho = J_2/J_1$. The straight lines for $\rho > 1$ are exponential fits and the curves for $\rho = 1$ are power-law fits.

is possible. The most plausible scenario in 2D is that the behaviors found here are due to weak attractive interactions between a spinon and an anti-spinon—as would in fact be expected based on the DQC theory, where interactions are mediated by a gauge field (but the sign of the effective spinon-spinon interactions is not immediately clear). Note that we have only studied the lowest $S = 1$ state, and in higher states the kinetic energy should overcome the weak attraction, leading to essentially independent spinons, as found when comparing the critical J - Q model with a gas of free bosonic $S = 1/2$ excitations [24].

In the simple RVB spin liquid, we also found weak attractive interactions, but in this case the spinons are small. The differences between the RVB liquid and the critical J - Q_3 model should be due to the fact that the spin correlations decay exponentially in the former (and there is a spin gap), while they have a power-law decay the latter. Both models exhibit algebraic dimer correlations, which should be responsible for the residual spinon interactions. In the 1D case, full deconfinement can be seen thanks to repulsive interactions, although the critical spinons themselves are not small particles (as in the 2D J - Q_3 model), being instead marginally localizable objects described by power-law overlaps. Still, it is rigorously known that these marginal particles do propagate as individual degrees of freedom [8].

Our results suggest that the critical J - Q_3 model and other related systems (generic Néel–VBS critical points) are close 2D analogues to the 1D critical spin chains, with the differences essentially due to the different topological aspects of the spinons; vortices versus kink solitons.

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